PLENARY LECTURE

MOAam 08:00 **Airborne Cell Chemistry**; Sabina Santesson; Thomas Johansson; Johan Nilsson; Eva Degerman; Patrik Rorsman; Peter Viberg; Peter Spégel; **Staffan Nilsson**; *Lund University, Lund, Sweden*

MONDAY MORNING ORAL SESSION MOA
PROTEOMICS: NEW TECHNOLOGIES, Michael Baldwin, Chair

MOAam 10:15 **Rapid, Sensitive and Quantitative Measurements of Proteomes**; Richard D. Smith; Ljiljana Pasa-Tolic; Mary S. Lipton; Timothy D. Veenstra; Richard Harkewicz; Yufeng Shen; Gordon A. Anderson; Harold R. Udseth; Christophe Masselon; Mikhail E. Belov; Thomas P. Conrads; Lingjun Li; *Pacific Northwest National Laboratory, Richland, WA*

MOAam 10:35 **Rapid, Automatic Identification of Proteins Utilizing a Novel MALDI-Ion Trap Mass Spectrometer**; Andrew N. Krutchinsky[1]; Markus Kalkum[1]; Ronald C. Beavis[2]; Brian T. Chait[1]; *[1]The Rockefeller University, New York, NY; [2]Proteometrics, LLC, New York, NY*

MOAam 10:55 **Regionalization of Epididymal Proteins in Tissue Sections by Mass Spectrometry and Correlation with mRNA Expression;** Pierre Chaurand; Sophie Fouchecourt; Beverly DaGue; Yoshihiko Araki; Marie-Claire Orgebin-Crist; Richard M. Caprioli; *Vanderbilt University, Nashville, TN*

MOAam 11:15 **Top Down Characterization of Unique Protein-protein Complex and Posttranslational Modifications by High Resolution Tandem Mass Spectrometry**; Ying Ge; Jun Xi; Brian G. Lawhorn; Tadhg P. Begley; Fred W. McLafferty; *Cornell University, Dept. of Chem., Ithaca, NY*

MOAam 11:35 **High Throughput Liquid Phase Microseparation - MALDI/MS for Proteomics**; Barry L. Karger; Ping Hu; Tomas Rejtar; Jan Preisler; Frantisek Foret; *Northeastern University, Boston, MA*

MOAam 11:55 **Reliable Protein Identification from Stained or Unstained 2D Gels Using High Throughput MALDI TOF/TOF MS;** A.L. Burlingame[1]; Lan Huang[1]; Katherine E. Williams[1]; Carina Sihlbom[1]; Katalin F. Medzhiradszky[1]; Maria Pallavicini[1]; Jennifer M. Campbell[2]; Peter Juhasz[2]; Steven A. Martin[2]; Marvin L. Vestal[2]; Michael A. Baldwin[1]; *[1]University of California, San Francisco, CA; [2]Applied Biosystems, Framingham, MA*

MONDAY MORNING ORAL SESSION MOB
IONIZATION PROCESSES, Renato Zenobi, Chair

MOBam 10:15 **Heating to Maximize AP-MALDI Performance: Evidence for Desolvation**; Ryan M. Danell; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*

MOBam 10:35 **Aspects of Photoionization and Energy Pooling Ionization Mechanisms in UV-MALDI**; Richard Knochenmuss; Qiong Lin; Patrick Setz; Renato Zenobi; *Swiss Federal Inst. of Technology, Zurich, Switzerland*

MOBam 10:55 **Observation and Stability of Non-Specific Small Size Peptide Cluster Ions in MALDI/TOFMS**; Vincent Livadaris; Jean-Claude Blais; Jean-Claude Tabet; *CNRS, Université Pierre et Marie Curie, Paris, France*

MOBam 11:15 **Ion Formation in IR-MALDI**; Christoph Menzel; Andreas Rohlfing; Stefan Berkenkamp; Hanno Ehring; Franz Hillenkamp; Klaus Dreisewerd; *Institute of Medical Physics & Biophysics, Muenster, Germany*

MOBam 11:35 **Stabilization of Anion Attachment in Negative Ion Electrospray Mass Spectrometry**; Yang Cai; Richard B. Cole; *University of New Orleans, New Orleans, LA*

MOBam 11:55 **The Effect of Analyte Affinity for the Droplet Surface on the Fraction of Analyte Charged during the Electrospray Ionization Process**; Nadja B. Cech; Christie G. Enke; *University of New Mexico, Albuquerque, NM*

MONDAY MORNING ORAL SESSION MOC
FT-ICR MS INNOVATIONS, Gökhan Baykut, Chair

MOCam 10:15 **Overview of FT-ICR MS Innovations**; Alan G. Marshall; *National High Magnetic Field Laboratory, Tallahassee, FL*

MOCam 10:35 **Charge-Changing Reactions and their Influence on the Ion Motion in an ICR Trap**; Alexander Herlert; Lutz Schweikhard; Manuel Vogel; *Inst. f. Physik, University of Mainz, Mainz, Germany*

MOCam 10:55 **Mass-Selective External Ion Accumulation for Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Christopher L. Hendrickson; John P. Quinn; Mark R. Emmett; Alan G. Marshall; *National High Magnetic Field Laboratory, Tallahassee, FL*

MOCam 11:15 **A New MALDI-FTMS Ion Source Design for Stabilization of Metastable Fragmentation by High Pressure Collisional Cooling**; Peter B. O'Connor; Ekaterina Mirgorodskaya; Catherine E. Costello; *Boston University, Boston, MA*

MOCam 11:35 **Intermediate Pressure MALDI FT-ICR Source for Proteomics**; Ansgar Brock; Christopher M. Shaw; Eric C. Peters; Christer Ericson; David M. Horn; *GNF, San Diego, CA*

MOCam 11:55 **Large Emitting Area Electron Gun for Electron Capture Dissociation in Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Youri O. Tsybin; Per Hakansson; *Angstrom Laboratory, Uppsala University, Uppsala, Sweden*

MONDAY MORNING ORAL SESSION MOD
LC/MS HIGH FLOW RATE & HIGH THROUGHPUT,
Dorothy J. Phillips, Chair

MODam 10:15 **Achieving a Mass Sensitive Response from the Electrospray Process in the Milliliter per Minute Flow Regime**; Peter Kovarik; Raymond Jong; Timothy Hoffman; Hassan Javaheri; Clevys Monasterios; Thomas Covey; *Applied Biosystems/ MDS SCIEX, Concord, Canada*

MODam 10:35 **What Limits Productivity in High Flow Fast LC/MS?**; Mark J. Hayward; James L. Munson; Grainne Conneely; Leonard O. Hargiss; *Novartis Pharmaceuticals, Summit, NJ*

MODam 10:55 **Maximizing Throughput in LC-MS**; Uwe D. Neue[1]; Claude Mallet[1]; Ziling Lu[1]; Yung-Fong Cheng[2]; *[1]Waters Corporation, Milford, MA; [2]TransForm Pharmaceuticals, Waltham, MA*

MODam 11:15 **Designing Walk Up LC/MS Systems to Match the Speed of High Throughput Purification Methods: Use of Monolithic Chromatography**; Andrew J. Organ; Brooke L. Daniel; *GlaxoSmithKline Pharmaceuticals, Harlow, UK*

MODam 11:35 **Fast-flow LC/MS Characterization of Proenkephalin A-Derived Peptides from Bovine Adrenal Medulla**; Haiping Wang; Chhabil Dass; *The University of Memphis, Memphis, TN*

MODam 11:55 **Development and Validation of a High Throughput Clinical Assay Using a Semi-Automated 96-Well Extraction Combined with Normal Phase LC/MS/MS and Subsequent Transfer to CRO;** Hesham Ghobarah[1]; John D. Laycock[1]; Krys J. Miller[1]; Ridha Nachi[2]; Christine Sartwell[2]; *[1]Amgen Inc., Thousand Oaks, CA; [2]MDS Pharma Services, Lincoln, NE*

MONDAY MORNING ORAL SESSION MOE
ENVIRONMENTAL CHEMISTRY, Peter Palmer, Chair

MOEam 10:15 **Environmental Monitoring Using Membrane Introduction Combined with Proton-Transfer-Reaction Mass Spectrometry (PTR-MS);** Michael L. Alexander[1]; Werner Lindinger[2]; Elena Boscaini[2]; Peter Prazeller[2]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Institut fur Ionenphysik, Innsbruck, Austria*

MOEam 10:35 **Desorption Chemical Ionization MIMS: A New Method for the Direct Detection of Contaminants in Water;** Tenna Aggerholm; Frants R. Lauritsen; *Odense University - SDU, Odense, Denmark*

MOEam 10:55 **Autonomous In-Water Chemical Analysis Using Membrane Introduction Mass Spectrometry;** David P. Fries; R. Timothy Short; Gottfried Kibelka; Michael L. Kerr; *University of South Florida, COT, St. Petersburg, FL*

MOEam 11:15 **Chemical and Toxicological Evaluation of Chlorinated and Ozonated-Chlorinated Drinking Water: A Collaboration of the Four National Labs of the U.S. EPA;** Susan D. Richardson[1]; Alfred D. Thruston, Jr.[1]; Thomas F. Speth[2]; Richard J. Miltner[2]; Glenn Rice[2]; Kathleen M. Schenck[2]; Stuart W. Krasner[3]; Howard S. Weinberg[4]; Linda K. Teuschler[2]; Jane Ellen Simmons[5]; *[1]U.S. Environmental Protection Agency, Athens, GA; [2]U.S. Environmental Protection Agency, Cincinnati, OH; [3]Metropolitan Water District of So. Calif, La Verne, CA; [4]University of North Carolina, Chapel Hill, NC; [5]U.S. Environmental Protection Agency, RTP, NC*

MOEam 11:35 **Structural Characterization of Individual Compounds within Complex Organic Mixtures Using High Resolution Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FTICR MS);** Elizabeth B. Kujawinski; Patrick G. Hatcher; Michael A. Freitas; *The Ohio State University, Columbus, OH*

MOEam 11:55 **A Comparison of Real-Time Single Particle Analysis of Ambient Aerosols During Fog Events;** Jeffrey R. Whiteaker; Kimberly A. Prather; *University of California, Riverside, CA*

MONDAY AFTERNOON ORAL SESSION MOA
ION ACTIVATION/DISSOCIATION, Roman Zubarev, Chair

MOApm 3:00 ***De Novo* Sequence Identification and Characterization of Intact Proteins via CID with a Quadrupole-TOF Mass Spectrometer;** Jennifer F. Nemeth; Jason C. Rouse; Hubert A. Scoble; *Genetics Institute, Andover, MA*

MOApm 3:20 **An Investigation of Parameters Controlling Collision Induced Dissociation in a MALDI Time of Flight/Time of Flight Instrument;** Jennifer M. Campbell; Kevin M. Hayden; Marvin L. Vestal; *Applied Biosystems, Framingham, MA*

MOApm 3:40 **Thermally-Assisted Infrared Multiphoton Photodissociation in a Quadrupole Ion Trap;** Anne H. Payne; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*

MOApm 4:00 **High Sensitivity Electron Capture Dissociation Tandem Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for Structural Characterization of Peptides and Glycopeptides;** Kristina Hakansson[1]; Carol L. Nilsson[2]; Mark R. Emmett[1]; Christopher L. Hendrickson[1]; Alan G. Marshall[1]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Goteborg University, Goteborg, Sweden*

MOApm 4:20 **Novel Electron-induced Activation Techniques for Peptide Ions;** Bogdan A. Budnik; Kim F. Haselmann; Roman A. Zubarev; *Dept. Chem., University of Southern Denmark, Odense, Denmark*

MOApm 4:40 **Optimization of the Signals for the High Mass Fragment ions (m/z > 3000) Produced by In-source Fragmentation in Delayed Extraction MALDI-TOFMS;** Viswanatham Katta; Edward T. Chin; Reed J. Harris; *Genentech Inc., S. San Francisco, CA*

MONDAY AFTERNOON ORAL SESSION MOB
REACTIONS OF TRAPPED IONS: ORGANIC COMPOUNDS, CLUSTERS, METALS, Hilkka Kenttämaa, Chair

MOBpm 3:00 **Gas Phase Reactions of Borane and Trimethylborate with Amino Acids, Peptides, and Peptide Derivatives;** Scott Gronert[1]; Renee Huang[1]; Richard A. J. O'Hair[2]; *[1]San Francisco State University, San Francisco, CA; [2]University of Melbourne, Melbourne, Australia*

MOBpm 3:20 **Double Resonance and Self-Ionization for Studying Precursor and Transient Ions Involved in Ion-Molecule Reactions;** Marina V. Da Silva; Marie-Claude Perlat; Jean-Claude Tabet; *Université Pierre et Marie Curie (LCSOB), Paris, France*

MOBpm 3:40 **Gas Phase Ion-Molecule Chemistry of Yttrium and Lanthanum Carbide Cluster Cations with Benzene and Related Molecules;** Gary D. Willett; Adriana Dinca; Keith J. Fisher; Rui Zhang; *The University of New South Wales, Sydney, Australia*

MOBpm 4:00 **Study of Competing Reactions: Direct Dissociation vs. Isomerization Reactions of the $C_8H_8O_2^{\cdot+}$ Ions Formed from Methyl Benzoate;** Scott M. Peterman; Guido F. Verbeck IV; David H. Russell; *Texas A&M University, College Station, TX*

MOBpm 4:20 **Distonic *meta*-Benzyne Ions: Substituent Effects on Reactivity;** Jason M. Price; Hilkka I. Kenttämaa; *Purdue University, West Lafayette, IN*

MOBpm 4:40 **Determination of Barriers to Methyl Cation Transfer Reactions from Fourier Transform Ion Cyclotron Resonance Kinetics Experiments;** Terrance B. McMahon; Travis D. Fridgen; *University of Waterloo, Waterloo, ON; Canada*

MONDAY AFTERNOON ORAL SESSION MOC
NOVEL USES OF MASS SPECTROMETRY, Gary Siuzdak, Chair

MOCpm 3:00 **Investigating Intact Viruses with Charge-Detection MS and Ion Mobility;** W. Henry Benner[1]; Christopher A. Hack[1]; Joseph A. Traina[2]; *[1]Lawrence Berkeley National Laboratory, Berkeley, CA; [2]Berlex Biosciences, Inc., Richmond, CA*

MOCpm 3:20 **Mass Spectrometric Identification of Pigments and Media in Modern Paintings;** Jaap J. Boon[1]; Nicolas Wyplosz[1]; Tom Learner[2]; Ron Heeren[1]; *[1]FOM Instititute AMOLF, Amsterdam, The Netherlands; [2]Tate Gallery, London, UK*

MOCpm 3:40 **Analysis and Purification of Hydrophobic Peptides Using SFC/MS and Preparative SFC;** Michael J. Greig; William Farrell; Haitao Li; Manuel C. Ventura; *Pfizer Global R&D - La Jolla, San Diego, CA*

MOCpm 4:00 **DIOS-MS Identification of Polymer Traces: Forensic Applications**; Robert D. Blackledge[1]; John J. Thomas[2]; Zhouxin Shen[3]; *[1]Naval Criminal Investigative Service, San Diego, CA; [2]Scripps Research Institute, La Jolla, CA; [3]University of California San Diego, La Jolla, CA*

MOCpm 4:20 **How Small Can We Go? Assaying Single Organelles and Release from a Single Cell Using Mass Spectrometry**; Jonathan Sweedler; Stanislav Rubakhin; Brian Monroe; Jason Page; Lingjun Li; *University of Illinois, Urbana, IL*

MOCpm 4:40 **A Novel Method for the Analysis of Complex Biological Protein Mixtures Using Electrospray Ionization Mass Spectrometry Combined with Ion/Ion Chemistry**; Jonathan L. Bundy[1]; Nathan C. VerBerkmoes[1]; James L. Stephenson Jr. [1]; Scott A. McLuckey[2]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]Chem. Dept., Purdue University, West Lafayette, IN*

MONDAY AFTERNOON ORAL SESSION MOD
CARBOHYDRATE SEQUENCING, Julie Leary, Chair

MODpm 3:00 **A Rapid Mass Spectrometry Method for Determining Intra-Species Diversity in Oligosaccharides**; Yongming Xie[1]; Ken Tseng[1]; Armando Romero[1]; Jennifer Cruz[1]; Jerry L. Hedrick[2]; Carlito B. Lebrilla[1]; *[1]Dept. of Chemistry, University of California, Davis, CA; [2]MCB Section, University of California, Davis, CA*

MODpm 3:20 **Characterization of LOS from Neisseria Gonorrhoeae**; Michael D. Leavell[1]; Futoshi Konishi[2]; Michiko Hirose[2]; Ryohei Yamasaki[2]; Julie A. Leary[1]; *[1]University of California, Berkeley, CA; [2]Tottori Univeristy, Tottori, Japan*

MODpm 3:40 **Utilizing the Sialic Acid Pathway for Metabolic Engineering of Cell Surface Glycoforms in Haemophilus Ducreyi**; Birgit Schilling[1]; Scarlett Goon[2]; Sara P. Gaucher[1]; Nicole M. Samuels[2]; Julie A. Leary[2]; Carolyn R. Bertozzi[2]; Bradford W. Gibson[3]; *[1]Buck Institute for Age Research, Novato, CA; [2]University of California, Berkeley, CA; [3]University of California, San Francisco, CA*

MODpm 4:00 **Tandem Mass Spectrometric Analysis of Glycosaminoglycan Oligosaccharides**; Joseph Zaia; Joseph E. McClellan; Catherine E. Costello; *Boston University School of Medicine, Boston, MA*

MODpm 4:20 **Fragmentation of Native and Peracetylated Oligosaccharides in PSD MALDI-TOF and CID MALDI Q-TOF MS**; Marko Jovanovic[1]; Matthew Willetts[2]; Richard Tyldesley[2]; Jeff Brown[2]; Jasna Peter-Katalinic[1]; *[1]Institute for Medical Biophysics, Muenster, Germany; [2]Micromass UK Limited, Manchester, UK*

MODpm 4:40 **Detailed Structural Characterization of a Series of Glycoside Resins Using Mass Spectrometry**; Douglas M. Sheeley[1]; Curtis Barnes[3]; Bryan J. Fritz[2]; Catherine M. Kolf[2]; Lewis K. Pannell[2]; Kirk P. Manfredi[3]; *[1]Nat. Center for Research Resources, NIH, Bethesda, MD; [2]NIDDK, NIH, Bethesda, MD; [3]Dept. of Chemistry, University of Northern Iowa, Cedar Falls, IA*

MONDAY AFTERNOON ORAL SESSION MOE
ENVIRONMENTAL CONTAMINANTS,
Don Betwoski & Ed Furlong, Chairs

MOEpm 3:00 **"Emerging" Pollutants, Mass Spectrometry, and Communicating Science: Pharmaceuticals in the Environment**; Christian G. Daughton; *U.S. Environmental Protection Agency, Las Vegas, NV*

MOEpm 3:20 **Analysis of Natural and Synthetic Estrogens in Water Using ESI/LC/MS Coupled with SPE**; John E. George; Yongtao Li; Earl M. Hansen; Jerry J. Thoma; *Environmental Health Laboratories, South Bend, IN*

MOEpm 3:40 **Analysis of Trace Levels of Sulfonamide and Tetracycline Antibacterials in Ground and Surface Water Using Liquid Chromatography/Mass Spectrometry**; E. Michael Thurman; Michele E. Lindsey; *U.S. Geological Survey, Lawrence, KS*

MOEpm 4:00 **MALDI-TOF-MS Detection of Aerosolized Bacterial Spores in the Presence of Environmental Clutter**; Andrew B. Feldman[1]; William R. Allman[1]; Micah A. Carlson[1]; Bernard F. Collins, Timothy J. Cornish[1]; Scott A. Ecelberger, Douglas L. Lewis[1]; Jeffrey S. Lin[1]; Michael P. McLoughlin[1]; Fernando J. Pineda[1]; L. Pitt, M. West[2]; Peter F. Scholl[1]; James T. Velky[1]; Wayne A. Bryden[1]; *[1]Johns Hopkins University/Applied Physics Laboratory, Laurel, MD; [2]U.S. Army Med. Res. Inst. Infect. Dis., Ft. Detrick, MD*

MOEpm 4:20 **Determination of Halogenated Derivatives of Alkyl Phenol Ethoxylates in Wastewaters and Sludges by SPE-LC/MS**; Damia Barcelo[1]; Mira Petrovic[1]; Francesc Ventura[2]; *[1]IIQAB-CSIC, Barcelona, Spain; [2]ABGAR, Barcelona, Spain*

MOEpm 4:40 **Concentrations and Spatial Variations of Polybrominated Diphenyl Ethers in Air, Fish, Sediment, and Baby's Blood from the Northeastern United States**; Ronald A. Hites; Nathan G. Dodder; Bo Strandberg; *Indiana University, Bloomington, IN*

PLENARY LECTURE

TOAam 8:00 **Award for a Distinguished Contribution in Mass Spectrometry: George C. Stafford**, *Thermo Finnigan, San Jose, CA*

TUESDAY MORNING ORAL SESSION TOA
BIOMACROMOLECULAR COMPLEXES,
Kenneth Standing, Chair

TOAam 10:15 **A Comprehensive Proteomic Analysis of Human Cilia: Identification of Novel Ciliary Components**; Robert K. Blackburn[1]; Lawrence E. Ostrowski[2]; William A. Burkhart[1]; Mary B. Moyer[1]; Daniela M. Schlatzer[1]; Kristen M. Radde[2]; Richard C. Boucher[2]; M. Arthur Moseley[1]; *[1]Glaxo SmithKline, RTP, NC; [2]University of North Carolina, Chapel Hill, NC*

TOAam 10:35 **Characterization of the Dimerization Motif of Sulfotransferases by Site-directed Mutagenesis, Crosslinking and Mass Spectrometry**; Evgeniy V. Petrotchenko; Christoph H. Borchers; Lars C. Pedersen; Kenneth B. Tomer; Masahiko Negishi; *NIEHS, RTP, NC*

TOAam 10:55 **Dissociation Pathways of Macromolecular Complexes**; Chalotte L. Hanson; Margaret G. McCammon; Frank Sobott; Helena Hernandez; Carol V. Robinson; *Oxford Centre for Molecular Sciences, Oxford, UK*

TOAam 11:15 **Mass Spectrometric Analysis of a UV-Cross-linked Protein-DNA Complex - Tryptophan 88 of E. coli SSB Cross-Links to DNA**; Hanno Steen; Jørgen Petersen; Matthias Mann; Ole N. Jensen; *University of Southern Denmark, Odense, Denmark*

TOAam 11:35 **Understanding Cellular Processes: Identification of Proteins in Functional Complexes Using Different Mass Spectrometric Approaches**; Manfred Raida; Markus Boesche; Volker Gnau; Bernhard Kuster; Paola Grandi; Andreas Bauer; Gitte Neubauer; *CellZome GmbH, Heidelberg, Germany*

TOAam 11:55 **ESI-MS of Noncovalent DNA-Protein Interactions**; Jennifer L. Beck[1]; Amit Kapur[1]; Susan E. Brown[2]; Nicholas E. Dixon[2]; Margaret M. Sheil[1]; *[1]University of Wollongong, Wollongong NSW, Australia; [2]Australian National University, Canberra ACT, Australia*

TUESDAY MORNING ORAL SESSION TOB
ION ACTIVATION/DISSOCIATION: SMALL MOLECULES, Mary T. Rodgers, Chair

TOBam 10:15 **A Direct Experimental Measurement of the Energy Deposition Function in Collisions**; Peter B. Armentrout; Felician Muntean; *Chemistry Department, University of Utah, Salt Lake City, UT*

TOBam 10:35 **Internal Energy Control in Activated Ion Dissociation Experiments**; Ron M. A. Heeren[1]; Xinghua Guo[1]; Marc C. Duursma[1]; Laszlo Drahos[2]; Karoly Vekey[2]; *[1]FOM AMOLF, Amsterdam, The Netherlands; [2]CRIC, Budapest, Hungary*

TOBam 10:55 **Resonance Excitation in Flow-Through RF-Only Ion Guides**; Raymond E. March; Igor Galetich; Chunyan Hao; *Water Quality Centre, Trent University, Peterborough, Canada*

TOBam 11:15 **Collision-Induced Dissociation of the Hypervalent Anion PCl_6^-**; Lee S. Sunderlin; Catherine E. Check; Thomas M. Gilbert; *Northern Illinois University, DeKalb, IL*

TOBam 11:35 **Modeling Deoxyribose Radical Intermediates by Neutralization Reionization Mass Spectrometry and Computational Chemistry**; Vivekananda Shetty; Frantisek Turecek; *University of Washington, Seattle, WA*

TOBam 11:55 **Evaluation of Relative Binding Energies of Pyridyl Ligand/Metal Complexes**; Jennifer S. Brodbelt[1]; Mary B. Satterfield[2]; *[1]University of Texas, Austin, TX; [2]NIST, Gaithersburg, MD*

TUESDAY MORNING ORAL SESSION TOC
DESIGNS FOR THE FUTURE, Richard D. Smith, Chair

TOCam 10:15 **A Hybrid Quadrupole Ion Trap - Fourier Transform Mass Spectrometer: A New Tool for Proteomics**; John E. P. Syka[1]; George C. Stafford Jr.[2]; Stevan Horning[3]; Jeffrey Shabanowitz[1]; Donald F. Hunt[1]; Jarrod A. Marto[1]; *[1]University of Virginia, Charlottesville, VA; [2]ThermoFinnigan LLC, San Jose, CA; [3]ThermoFinnigan GmbH, Bremen, Germany*

TOCam 10:35 **Fluidic Pulsing System as an Ultra Fast Serial Sample Introduction System**; Thomas Covey[1]; Adam Weiss[2]; Ray Jong[1]; *[1]Applied Biosystems/MDS SCIEX, Concord, Canada; [2]De.Vice Engineering Inc., Pickering, Canada*

TOCam 10:55 **Piezoelectric Source for Single Droplet Mass Spectrometry**; Travis Berggren; Michael Westphall; Mark Scalf; Lloyd M. Smith; *University of Wisconsin, Madison, WI*

TOCam 11:15 **A Novel Design for Sheathless Electrospray and Nanospray for Low Flow and High Sensitivity Applications in Mass Spectrometry**; Magnus Wetterhall; Stefan Nilsson; Karin Markides; Jonas Bergquist; *Dept. Anal. Chem., Uppsala University, Uppsala, Sweden*

TOCam 11:35 **Design and Applications of a New High Resolution Triple Quadrupole Mass Spectrometer**; Alan E. Schoen; Jean-Jacques Dunyach; Hans Schweingruber; Steve Hurwitz; Wayne Dewey; Bill Siebert; Nigel Gore; Rex Heller; Phil Fong; Eugene Zhuk; Dennis Taylor; Clay Campbell; *ThermoFinnigan, San Jose, CA*

TOCam 11:55 **Annotating the Genome by Mass Spectrometry: Exon Mapping with MS^2 Data**; Markus Kalkum[1]; Brian T. Chait[1]; Ronald C. Beavis[2]; *[1]The Rockefeller University, New York, NY; [2]ProteoMetrics, LLC, New York, NY*

TUESDAY MORNING ORAL SESSION TOD
GLYCOCONJUGATES, Steven B. Levery, Chair

TODam 10:15 **Mass Spectrometry Applied to the Analysis of Glycoproteins**; Nelly Viseux; *Biogen, Inc., Cambridge, MA*

TODam 10:35 **Site-Mapping and Structural Characterization of the Glycosylation of PME Mutants by MALDI-MS and ESI-MS on a Q-TOF**; Maria R. Esteban Warren[1]; Harry Kester[2]; Jacques Benen[2]; Lin Lin[1]; Jaap Visser[2]; Carl Bergmann[1]; Ron Orlando[1]; *[1]University of Georgia, Athens, GA; [2]Wageningen Agricultural University, Wageningen, The Netherlands*

TODam 10:55 **Analysis of Protein O-Fucosylation Using Nano-ESI Q-TOF Mass Spectrometry**; Boris Macek[1]; Anne Gonzalez de Peredo[2]; Dominique Klein[2]; Jan Hofsteenge[2]; Jasna Peter-Katalinic[1]; *[1]Institute for Med. Physics a. Biophysics, Muenster, Germany; [2]Friedrich Miescher Institute, Basel, Switzerland*

TODam 11:15 **Mutual Differentiation of Cationized Enantiomeric and Diastereomeric Alcool/Carbohydrates Complexes by ESI/ITMS**; Valérie Carlesso; Françoise Fournier; Jean-Claude Tabet; *Université Pierre et Marie Curie, Paris, France*

TODam 11:35 **Sheathless CE/ESI-QTOF-MS Interface for Identification of Carbohydrates**; Alina Zamfir; Jasna Peter-Katalinic; *Medical Physics and Biophysics, Münster, Germany*

TODam 11:55 **Identification and Analysis by ESI-MS of Glycoinositolphospholipids from Mammalian Cell-Derived Stages of Trypanosoma Cruzi**; Igor C. Almeida[1]; Michael A. J. Ferguson[2]; *[1]University of Sao Paulo, Parasitology, Sao Paulo, SP, Brazil; [2]University of Dundee, Biochemistry, Dundee, Scotland, UK*

TUESDAY MORNING ORAL SESSION TOE
NOVEL MS APPROACHES IN THE DRUG METABOLISM ENVIRONMENT, Meg Annan, Chair

TOEam 10:15 **Drug Metabolite Characterization by Matrix Assisted Laser Desorption Ionisation/Time of Flight-Mass Spectrometry (MALDI/TOF-MS)**; Daniel J. Weston[1]; Nigel Clarke[1]; Kathleen Cox[1]; Walter Korfmacher[1]; Steve Preece[2]; Jose Castro-Perez[2]; Richard Tyldesley[2]; *[1]Schering Plough Research Institute, Kenilworth, NJ; [2]Micromass UK Limited, Manchester, UK*

TOEam 10:35 **Simultaneous Sample Measurement for High-Throughput Mass Spectrometry**; Robert B. Cody; *JEOL USA, Inc., Peabody, MA*

TOEam 10:55 **Capillary LC/MS and LC/MS/MS Strategies Applied to High Throughput Metabolic Structure Elucidation in Drug Discovery**; Robyn A. Rourick[1]; Gary A. Valaskovic[2]; Daniel B. Kassel[1]; Mike S. Lee[3]; · *[1]DuPont Pharmaceuticals Research Laboratories, San Diego, CA; [2]New Objective, Inc., Cambridge, MA; [3]Milestone Development Services, Newtown, PA*

TOEam 11:15 **The Use of Accelerator Mass Spectrometry (AMS) to Investigate the Circulating Metabolites of Potential New Drugs**; Angus Nedderman[1]; Gill Allan[1]; Mark Savage[1]; Rob Webster[1]; Don Walker[1]; Daniel Leong[2]; Colin Garner[2]; *[1]Pfizer Global Research and Development, Sandwich, UK; [2]CBAMS Limited, York, UK*

TOEam 11:35 **Hyphenation Spectroscopy: Online Combination of LC-NMR/MS as a Novel Approach in Structure Elucidation**; Herbert Thiele[1]; Michael Biernacki[1]; Manfred Spraul[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Analytik GmbH, Karlsruhe, Germany*

TOEam 11:55 **Automated Product Ion Interpretation for Metabolite Identification**; Richard C. King; *Merck & Co., Inc, West Point, PA*

TUESDAY AFTERNOON ORAL SESSION TOA
PROTEOMICS: ALTERNATIVES TO 2-D GELS,
Lewis Pannell, Chair

TOApm 3:00 **The Trouble with 2D Gels for Proteome Analysis and Potential Alternatives**; Steven P. Gygi[1]; Ruedi Abersold[2]; *[1]Harvard Medical School, Boston, MA; [2]Institute for Systems Biology, Seattle, WA*

TOApm 3:20 **Development of an Integrated Analytical System for High-Throughput Quantitative Proteomic Analysis**; Timothy J. Griffin; Hookeun Lee; Ruedi Aebersold; *Institute for Systems Biology, Seattle, WA*

TOApm 3:40 **LC/MS and LC/MS/MS Strategies for Large-Scale Protein Identification and Quantification: A Combination of ESI-TOF and MALDI TOF-TOF Analysis**; Brian L Williamson[1]; Jason Marchese[1]; Nikita Khainovsky[1]; Peter Juhasz[1]; Steve Martin[1]; Michael D. Bond[2]; Robert Christian[2]; Thomas W. Hayes[2]; Scott D. Patterson[2]; *[1]Applied Biosystems - PRC, Framingham, MA; [2]Celera Genomics, Rockville, MD*

TOApm 4:00 **Proteomics of Histone Deacetylase Complexes in Budding Yeast and in Human**; Markus Kalkum; Andrew Krutchinsky; Jinsong Zhang; Denise Meagher; Robert G. Roeder; Brian T. Chait; *The Rockefeller University, New York, NY*

TOApm 4:20 **Integrated Microfluidic System Enabling Rapid Protein Separation, Digestion, and Identification for Proteome Analysis**; Cheng S. Lee[1]; Jinzhi Chen[1]; Jun Gao[1]; Deepa Mohan[1]; Richard D. Smith[2]; *[1]University of Maryland, College Park, MD; [2]Pacific Northwest National Laboratory, Richland, WA*

TOApm 4:40 **Proteomics of *Methanococcus jannaschii* with 100% Sequence Coverage**; Fanyu Meng; Benjamin J. Cargile; Andrew J. Forbes; Jeff R. Johnson; Neil L. Kelleher; *University of Illinois, Urbana, IL*

TUESDAY AFTERNOON ORAL SESSION TOB
IMMUNOLOGY, Amina S. Woods, Chair

TOBpm 3:00 **Characterization of STAM2 Using a New Method for Tyrosine Phosphorylation Analysis by Tandem Mass Spectrometry**; Hanno Steen[1]; Bernhard Küster[2]; Minerva Fernandez[1]; Akhilesh Pandey[1]; Matthias Mann[1]; *[1]BMB/University of Southern Denmark, Odense, Denmark; [2]MDS Protana A/S, Odense, Denmark*

TOBpm 3:20 **Comprehensive Analysis of MHC Class I Peptide Antigens from Cancer Cells by Mass Spectrometry;** Eilon Barnea; Ilan Beer; Renana Patuka; Tamar Ziv; Arie Admon; *Technion - Israel Institute of Technolog, Haifa, Israel*

TOBpm 3:40 **Guanidination of Class I Peptides Containing Lysine to Resolve Sequence Ambiguity**; Robert J. Cotter; Suzanne M. Ramirez; Mark J. Soloski; *Johns Hopkins School of Medicine, Baltimore, MD*

TOBpm 4:00 **Determination of Minor Histocompatibility Antigens by On-Line Nanoflow HPLC MicroESI Fourier Transform Mass Spectrometry**; Jennifer A. Caldwell[1]; Anthony G. Brickner[2]; Anne M. Evans[1]; Sahana Mollah[1]; Victor H. Engelhard[2]; Jeffrey Shabanowitz[1]; Donald F. Hunt[3]; *[1]Chemistry Dept. UVA, Charlottesville, VA; [2]Beirne Carter Center for Immunology UVA, Charlottesville, VA; [3]Chemistry and Pathology Depts UVA, Charlottesville, VA*

TOBpm 4:20 **Proteomics Screen for ER Resident Folding Factors**; Edwin P. Romijn[1]; Eelco van Anken[2]; Claudia Maggioni[2]; Roberto Sitia[3]; Ineke Braakman[2]; Albert J. R. Heck[1]; *[1]Biomolecular Mass Spectrometry, Utrecht, The Netherlands; [2]Bio-organic Chemistry, Utrecht, The Netherlands; [3]Laboratory of Mol. Immunology DIBIT-HSR, Milano, Italy*

TOBpm 4:40 **Development of an Immuno-Therapeutic Vaccine for Use in the Treatment of HPV Mediated Diseases**; Andy J. Tomlinson; Silvia S. Kwak; Wade M. Hines; Roman M. Chicz; *ZYCOS Inc, Lexington, MA*

TUESDAY AFTERNOON ORAL SESSION TOC
QUADRUPOLE ION TRAPS: NEW DESIGNS & APPLICATIONS, Joel H. Parks, Chair

TOCpm 3:00 **Ion Trap Mass Spectrometers: Designs and Potential Applications**; R. Graham Cooks; Wolfgang R. Plass; Garth E. Patterson; Andre N. Vilkov; Zoltan Takatis; *Purdue University, Dept. of Chemistry, West Lafayette, IN*

TOCpm 3:20 **Tandem Mass Spectrometry in a Miniature Cylindrical Ion Trap**; Thomas F. Meaker; Bert C. Lynn; *Mississippi State University, Mississippi State., MS*

TOCpm 3:40 **Modification of an Ion Trap for Real-Time Trapping of Nanoparticles--Megadalton and Beyond**; Peter T. A. Reilly; Ryan P. Rodgers; William B. Whitten; J. Michael Ramsey; *Oak Ridge National Lab, Oak Ridge, TN*

TOCpm 4:00 **Resonance Shifts in Quadrupole Excitation for n=0, K=1-4**; Bruce A. Collings[1]; Michael Sudakov[2]; Frank Londry[3]; Donald J. Douglas[4]; *[1]MDS Sciex, Concord, Ontario; [2]Ryazan Pedagogical University, Ryazan, Russia; [3]Pan Galactic Scientific, Peterborough, Canada; [4]University of British Columbia, Vancouver, Canada*

TOCpm 4:20 **IR Laser-Desorption / UV Resonant Two-Photon Ionisation Ion Trap Mass Spectrometry for Analysis of Polycyclic Aromatic Hyrdrocarbons**; August A. Specht; Michael W. Blades; *University of British Columbia, Vancouver, BC, Canada*

TOCpm 4:40 **Laser-Induced Fluorescence of Trapped FRET Ions**; Joseph T. Khoury; Sandra E. Rodriguez-Cruz; Joel H. Parks; *The Rowland Institute for Science, Cambridge, MA*

TUESDAY AFTERNOON ORAL SESSION TOD
DNA/RNA SEQUENCING, Margaret Sheil, Chair

TODpm 3:00 **Performance of the MALDI-QqTOF for DNA Analysis**; Stefan Berkenkamp[1]; Franz Hillenkamp[2]; Maciej Bromirski[3]; Werner Ens[3]; Ken Standing[3]; Alexander Loboda[4]; *[1]Sequenom GmbH, Hamburg, Germany; [2]University of Muenster, Muenster, Germany; [3]University of Manitoba, Winnipeg, Canada; [4]Sciex, Concord, Canada*

TODpm 3:20 **Identification of Pseudouridine in RNA by Matrix-Assisted Laser Desorption/Ionization (MALDI) Mass Spectrometry**; Kemberly G. Patteson; Patrick A. Limbach; *Louisiana State University, Baton Rouge, LA*

TODpm 3:40 **Structural Characterization of Carcinogen Modified DNA Adducts Using Enzymatic Digestion and MS/MS with MALDI/TOF/MS**; Sharon J. Shields; Chris A. Harvey; Karen Brown; Kenneth W. Turteltaub; *Lawrence Livermore National Laboratory, Livermore, CA*

TODpm 4:00 **An Electrospray Ionization Mass Spectrometry Method for Genotyping Single Nucleotide Polymorphisms**; Colleen K. Van Pelt; Sheng Zhang; Gary A. Schultz; *Advion BioSciences, Inc., Ithaca, NY*

TODpm 4:20 **Gas Phase Sequencing of PCR Amplicons Derived from Short Tandem Repeat Loci by ESI-FTICR-MS**; James C. Hannis; Allison P. Null; David C. Muddiman; *Virginia Commonwealth University, Richmond, VA*

TODpm 4:40 **Screening Entire Genes for Genetic Variants Using ESI/MS**; Chad C. Nelson; Lesa M. Nelson; Kenneth Ward; *EmerGen, Inc., Salt Lake City, UT*

TUESDAY AFTERNOON ORAL SESSION TOE
PHARMACEUTICALS: HIGH THROUGHPUT R-TO-D, Roy L. M. Dobson, Chair

TOEpm 3:00 **To "MUX" or Not To "MUX," That Is the Question**; Daniel B. Kassel[1]; Rongda Xu[1]; Tao Wang[1]; Andrew Brailsford[2]; Brian Smith[2]; *[1]DuPont Pharmaceuticals Research Laboratories, San Diego, CA; [2]Waters Corporation, Milford, MA*

TOEpm 3:20 **High Throughput Affinity Screening Based on High Performance Mass Spectrometry: Rapid and Automated Characterization of Noncovalent Complexes Comprised of Small Molecules Bound to Oligonucleotide or Protein Drug Targets**; Steven A. Hofstadler; Jared J. Drader; Kristin A. Sannes-Lowery; Sherilynn M. Manalili; Lendell L. Cummins; Yun Jiang; Richard H. Griffey; *Ibis Therapeutics - A Div. of Isis Pharm, Carlsbad, CA*

TOEpm 3:40 **Development and Applications of LC/MS for High Throughput Analytical Screening for "Accelerated" Compound Discovery**; Arkady I. Gusev; *Rohm and Haas Co, Spring House, PA*

TOEpm 4:00 **Is SFC/MS Ready for "Prime Time"? Screening of a Large and Diverse Library of Pharmaceutically Relevant Compounds Using Rapid SFC/MS, Including a New, Performance-Enhancing Mobile-Phase Additive**; J. David Pinkston[1]; Dong Wen[2]; Kenneth L. Morand[2]; Debra A. Tirey[2]; *[1]Procter & Gamble, Miami Valley Laboratories, Cincinnati, OH; [2]Procter & Gamble Pharmaceuticals, HCRC, Mason, OH*

TOEpm 4:20 **Current Approaches for High Throughput Bioanalytical and Prospects for the Future**; Steven H. Hoke, II[1]; John A. Tomlinson, II[1]; Renee D. Bolden[2]; Kenneth L. Morand[1]; J. David Pinkston[2]; Kenneth R. Wehmeyer[1]; *[1]The Procter & Gamble Company, Mason, OH; [2]The Procter & Gamble Company, Cincinnati, OH*

TOEpm 4:40 **A Parallel, Multiple On-line Extraction-Dual LC-MS-MS System for High Throughput Quantitative Bioanalysis in Drug Development**; Showchien Hsieh; John Dunn; *GlaxoSmithKline, RTP, NC*

PLENARY LECTURE

WOAam 8:00 **Biemann Medal: Peter B. Armentrout**, *University of Utah, Salt Lake City, UT*

WEDNESDAY MORNING ORAL SESSION WOA
PROTEIN CONFORMATIONS, Igor A. Kaltashov, Chair

WOAam 10:15 **Conformational Changes of the Ferric Uptake Regulation Protein upon Metal Activation and DNA Binding**; Anne Gonzalez de Peredo[1]; Christine Saint-Pierre[1]; Isabelle Michaud-Soret[2]; Eric Forest[1]; *[1]Institut de Biologie Structurale, Grenoble, France; [2]Departement de Recherche Fondamentale, Grenoble, France*

WOAam 10:35 **Determination of Disulfide Bonding Patterns in Cysteine-Rich Highly-Knotted Proteins**; Jack Throck Watson; Jianfeng Qi; Wei Wu; *Michigan State University, East Lansing, MI*

WOAam 10:55 **Protein-Membrane Interactions and Architecture Characterized by Combining Hydrogen/Deuterium Exchange and Mass Spectrometry**; Albert J. R. Heck; Jeroen A. A. Demmers; Esther van Duijn; J. Antoinette Killian; *Utrecht University, Utrecht, The Netherlands*

WOAam 11:15 **Ligand Binding in Hemoglobin and Myoglobin Evidence for Small Deviations between Gaseous and Solvated Protein Structures**; Keith A. Johnson; I. Jonathan Amster; *University of Georgia, Athens, GA*

WOAam 11:35 **Hydrogen Exchange Studies on Amyloid A-β Fibrils**; Indu Kheterpal[1]; Shaolian Zhou[2]; Ronald Wetzel[1]; Kelsey D. Cook[1]; *[1]University of Tennessee, Knoxville, TN; [2]Covance, Madison, WI*

WOAam 11:55 **A Mass Spectrometric Examination of the Quaternary Structure of the Nitric Oxide Synthase Oxygenase Domain**; Jeffrey C. Smith[1]; Steven P. Rafferty[2]; Timothy R. Croley[2]; Raymond E. March[2]; K. W. Michael Siu[1]; *[1]York University, Toronto, ON, Canada; [2]Trent University, Peterborough, ON, Canada*

WEDNESDAY MORNING ORAL SESSION WOB
MICROBES & PARASITES, Carol Nilsson, Chair

WOBam 10:15 **Characterization of Intact Microorganisms by Mass Spectrometry**; Catherine Fenselau; *University of Maryland, College Park, MD*

WOBam 10:35 **Mass Spectrometry, Bacteria, and Drug Discovery: Targeting Peptide Deformylase**; Rachel R. Ogorzalek Loo; Steve Dunham; Mike Kuhn; Eric Olson; Tod Holler; *Pfizer Global R&D, Ann Arbor, MI*

WOBam 10:55 **Analysis of Glycosylinositol Phosphorylceramides from Pathogenic Fungi by ESI-MS and Low-Energy Tandem ESI-MS/CID-MS of Lithium Adduct Ions**; Steven B. Levery[1]; Marcos S. Toledo[2]; Anita H. Straus[2]; Helio K. Takahashi[2]; *[1]University of Georgia, Athens, GA; [2]Universidade Federal de Sao Paulo, Sao Paulo, Brazil*

WOBam 11:15 **Identification of the Lactoferrin-Binding Outer Membrane Protein C (ompC) from *Escherichia coli* by an Affinity Crosslinking Approach**; Elisabet Gustafsson; Kajsa Thorön; Thomas Larsson; Karl-Anders Karlsson; Carol L Nilsson; *Göteborg University, Göteborg, Sweden*

WOBam 11:35 **Sequencing of Unknown Proteins from Plant Viruses by MALDI QqTOF Mass Spectrometry**; Yi-Min She[1]; Steve Haber[2]; Dallas L. Seifers[3]; Werner Ens[1]; Kenneth G. Standing[1]; *[1]Physics Dept., University of Manitoba, Winnipeg, Canada; [2]Agriculture & Agrifoods Canada, Winnipeg, Canada; [3]Kansas State University, Hays, KS*

WOBam 11:55 **Rapid Identification of Microorganisms by Matrix Assisted Laser Desorption/Ionisation Time of Flight Mass Spectrometry: An Inter-Laboratory Study;** Therese M. McKenna[1]; Martin S. Lunt[1]; Diane J. Dare[2]; Michelle M. Morgan[2]; John J. Bright[2]; Valerie Edwards-Jones[2]; Carrina J. Keys[3]; *[1]Micromass UK Ltd., Manchester, UK; [2]Manchester Metropolitan University, Manchester, UK; [3]NCTC, Central Public Health Laboratory, London, UK*

WEDNESDAY MORNING ORAL SESSION WOC
LIPIDS AND OXIDATIVE STRESS MARKERS,
Susan T. Weintraub, Chair

WOCam 10:15 **5-Oxo-7-Glutathionyl Eicosatrienoic Acid (FOG_7), A Novel Biologically Active Eicosanoid Catalysed by LTC_4 Synthase**; John M. Hevko; Robert C. Murphy; *National Jewish Medical Research Center, Denver, CO*

WOCam 10:35 **Vitamin C-Induced Decomposition of Lipid Hydroperoxides to Endogenous Genotoxins**; Seon Hwa Lee; Tomoyuki Oe; Ian A. Blair; *University of Pennsylvania, Philadelphia, PA*

WOCam 10:55 **Quantification of DNA Adducts Associated with Oxidative Stress**; Daniel R. Doerge; Mona I. Churchwell; Frederick A. Beland; *National Ctr for Toxicological Research, Jefferson, AR*

WOCam 11:15 **Protein Modification from Oxidation of Docosahexaenoate Phospholipids**; Xiaorong Gu[1]; Mingjiang Sun[1]; Bogdan G. Gugiu[1]; Masaru Miyagi[2]; Mary E. Rayborn[2]; Joe G. Hollyfield[2]; Robert G. Salomon[1]; John W. Crabb[2]; *[1]Case Western Reserve University, Cleveland, OH; [2]Cleveland Clinic Foundation, Cleveland, OH*

WOCam 11:35 **Lipid-Hydroperoxide-Mediated Covalent Modifications to Amino Acids**; Tomoyuki Oe; Seon Hwa Lee; Ian A. Blair; *University of Pennsylvania, Philadelphia, PA*

WOCam 11:55 **Fatty Acid Metabolite Analysis by Immunoassay and HPLC/MS/MS**; Gabriela Zurek; John W. Newman; Shirley Gee; Bruce D. Hammock; *University of California, Davis, CA*

WEDNESDAY MORNING ORAL SESSION WOD
ION STRUCTURES & ENERGETICS, K.W. Michael Siu, Chair

WODam 10:15 **The Structure and Energetics of Gas-Phase Biomolecules and Effects of Solvent**; Evan R. Williams; Rebecca A. Jockusch; Andrew S. Lemoff; Richard L. Wong; *University of California, Berkeley, CA*

WODam 10:35 **Fragmentation Energetics of Small Peptides from Multiple-Collision CID and SID in FT-ICR MS;** Julia Laskin; Eduard Denisov; Jean H. Futrell; *Pacific Northwest National Laboratory, Richland, WA*

WODam 10:55 **Structures and Energetics of Triply Protonated Bradykinin**; Yun Ling[1]; Christopher F. Rodriquez[1]; Yuzhu Guo[1]; Ivan K. Chu[2]; Gholamreza Javahery[2]; William W. Mak[3]; Alan C. Hopkinson[1]; K.W. Michael Siu[1]; *[1]York University, Toronto, Canada; [2]MDS SCIEX, Concord, Canada; [3]Seneca College, Toronto, Canada*

WODam 11:15 **Absolute Alkali Metal Ion Binding Energies of Substituted Uracils Determined by Threshold Collision-Induced Dissociation and *Ab Initio* Theory**; Mary T. Rodgers; *Wayne State University, Detroit, MI*

WODam 11:35 **Experimental Energy Barriers for Ethyl Cation Transfer Reactions**; Travis D. Fridgen; Terry B. McMahon; *University of Waterloo, Chemistry, Waterloo, Canada*

WODam 11:55 **Periodicities in the Kinetics of Oxidation Reactions of Lanthanide Cations with Nitrous Oxide and Oxygen**; Gregory K. Koyanagi; Diethard K. Bohme; *York University, Toronto, Canada*

WEDNESDAY MORNING ORAL SESSION WOE
ION MOBILITY, Martin F. Jarrold, Chair

WOEam 10:15 **Conformations and Energetics of Biopolomers in the Gas Phase Using Ion Mobility Methods: The Latest News**; Jennifer Gidden; Thomas Wyttenbach; Michael T. Bowers; *Department of Chemistry, University of Californai, Santa Barbara, CA*

WOEam 10:55 **Multidimensional High-Performance Liquid Chromatography/Ion Mobility/Time-of-Flight Mass Spectrometry (HPLC/IMS/TOFMS) Separations of Complex Biological Mixtures**; Catherine A. Srebalus Barnes; Amy E. Hilderbrand; Stephen J. Valentine; David E. Clemmer; *Indiana University, Bloomington, IN*

WOEam 11:15 **The Search for Novel Peptides: A New Application for Ion Mobility-Mass Spectrometry**; Brandon T. Ruotolo; Kent J. Gillig; Earle G. Stone; Guido F. Verbeck; David H. Russell; *Texas A&M University, College Station, TX*

WOEam 11:35 **Preliminary Ion Mobility Measurements in a Quadrupole Ion Trap**; Bert C. Lynn; *Mississippi State University, Mississippi State, MS*

WOEam 11:55 **Helix-Globule Transitions in Unsolvated Peptides**; Brian S. Kinnear; Matthew R. Hartings; Martin F. Jarrold; *Northwestern University, Evanston, IL*

WEDNESDAY MORNING ORAL SESSION WOF
MS OF POLYMERS, Charles McEwen, Chair

WOFam 10:15 **Ultra High Resolution MALDI-FTICR-MS for Block Length Distribution Analysis of Polystyrene-Block-Poly(Paramethyl Styrene);** Todd H. Mize[1]; Owen Terreau[2]; Adi Eisenberg[2]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]McGill University, Montreal, Canada*

WOFam 10:35 **MALDI-MS of Low-Molar Mass Polyethylene and Waxes;** Steffen M. Weidner; Gerhard Kuehn; Joerg F. Friedrich; *Federal Institute for Materials Research, Berlin, Germany*

WOFam 10:55 **MALDI MS of Saturated Hydrocarbon Polymers: Polyethylene and Other Polyolefins;** William E. Wallace; Charles M. Guttman; Bruno M. Fanconi; Barry J. Bauer; *Natl. Inst. Stand. Tech, Polym. Div., Gaithersburg, MD*

WOFam 11:15 **Mass Spectrometric Analysis of Poly(Methyl Methacrylate) (PMMA) Generated by Means of Atom Transfer Radical Polymerisation (ATRP);** Anthony T. Jackson[1]; Christopher D. Borman[2]; Derek J. Irvine[2]; Martin R. Green[3]; Robert H. Bateman[3]; *[1]Measurement Science Group, ICI plc, Middlesbrough, UK; [2]Ineos Acrylics, Middlesbrough, UK; [3]Micromass UK Ltd, Manchester, UK*

WOFam 11:35 **The Use of Functional and Chain-Extended Initiators in the Anionic Polymerization of Dienes;** Chrys Wesdemiotis[1]; Mark A. Arnould[1]; Tae H. Cheong[2]; Roderic P. Quirk[2]; *[1]The University of Akron, Chemistry, Akron, OH; [2]The University of Akron, Polymer Science, Akron, OH*

WOFam 11:55 **Analysis of Low-temperature Pyrolysis Products from Poly(tetrahydrofuran) and a PTHF-Based Polyurethane;** Robert P. Lattimer; *BFGoodrich Performance Materials, Brecksville, OH*

WEDNESDAY AFTERNOON ORAL SESSION WOA
PROTEIN-METAL AND PROTEIN LIGAND INTERACTIONS,
Peter J. Derrick, Chair

WOApm 3:00 **Metal-Protein Interactions: Contributions of Mass Spectrometry to Bioinorganic Chemistry;** Dan Fabris; *University of Maryland, Baltimore County, Baltimore, MD*

WOApm 3:20 **Reactions of Ferri- and Ferro-Cytochrome C Ions in the Gas Phase;** J. Mitchell Wells; Gavin E. Reid; Brian J. Engel; Peng Pan; Scott A. McLuckey; *Purdue University Department of Chemistry, West Lafayette, IN*

WOApm 3:40 **Dissociation Pathways, Kinetics and Energetics of Oligosaccharide-Protein Complexes in the Gas Phase;** Elena N. Kitova; David R. Bundle; John S. Klassen; *University of Alberta, Edmonton, Canada*

WOApm 4:00 **Investigation of Iron Biniding and Release from Transferrins by ESI MS;** Dmitry R Gumerov[1]; Anne B. Mason[2]; Igor A. Kaltashov[1]; *[1]University of Massachusetts, Amherst, MA; [2]University of Vermont School of Medicine, Burlington, VT*

WOApm 4:20 **Determination of Metal-Protein Complexes and Posttranslational Modifications by LC-(ESI-TOF)-MS;** Rannar Sillard[1]; Elo Eriste[1]; Olga Njunkova[2]; Lesja Pokras[2]; Hans Jörnvall[1]; Henrik Wadensten[3]; Staffan Renlund[3]; Peep Palumaa[2]; *[1]Dept. MBB, Karolinska Institute, Stockholm, Sweden; [2]Tallinn Technical University, Tallinn, Estonia; [3]Amersham Pharmacia Biotech, Uppsala, Sweden*

WOApm 4:40 **Structure Determination of Protein Noncovalent Complexes by Mass Spectrometry;** Joseph A. Loo; *Pfizer Global Research and Development, Ann Arbor, MI*

WEDNESDAY AFTERNOON ORAL SESSION WOB
DIAGNOSIS OF DISEASES, Stephen Naylor, Chair

WOBpm 3:00 **Keynote Lecture;** Michael M. Morris

WOBpm 3:20 **Development of Steroid Metabolic Profiling by Tandem Mass Spectrometry (MS/MS) for the Detection of Congenital Adrenal Hyperplasia (CAH);** Mark J. Magera[1]; Carla Z. Minutti[1]; Bruno N. Casetta[2]; Donald Zimmerman[1]; Piero Rinaldo[1]; Dietrich Matern[1]; *[1]Mayo Clinic, Rochester, MN; [2]Applied Biosystems, Monza, Italy*

WOBpm 3:40 **Rapid Analysis of Eicosanoids from Complex Matrices;** H. Robert Bergen III; Michael J. Murray; Edd L. Evans; Stephen Naylor; *Mayo Clinic, Rochester, MN*

WOBpm 4:00 **Mass Spectrometry on Track of Celiac Disease;** Petr Novak[1]; Petr Man[1]; Jana Novotna[2]; Vladimir Havlicek[2]; Karel Bezouska[1]; Zuzana Flegelova[3]; Ludmila Tuckova[2]; *[1]Dept. Biochemistry, Charles University, Prague, Czech Republic; [2]Institute of Microbiology, Prague, Czech Republic; [3]BIOPHARM, Jilove, Czech Republic*

WOBpm 4:20 **Proteome-Wide Post-Translational Modifications and Database Search Algorithms for Characterization of Intact *H. pylori*;** Plamen A. Demirev[1]; Jeffrey S. Lin[2]; Fernando J. Pineda[2]; Catherine Fenselau[1]; *[1]University of Maryland, College Park, MD; [2]Johns Hopkins University, Laurel, MD*

WOBpm 4:40 **Lipoproteomics;** Ronald D. Macfarlane[1]; Zachlyn N. Farwig[1]; Anna V. Melnichenko[1]; Catherine J. McNeal[2]; *[1]Texas A&M University, College Station, TX; [2]Scott & White Hospital, Temple, TX*

WEDNESDAY AFTERNOON ORAL SESSION WOC
TOF ANALYZER DEVELOPMENT, Bernhard Spengler, Chair

WOCpm 3:00 **Design and Performance of Improved MALDI TOF-TOF System;** Marvin L. Vestal; Jennifer M. Campbell; Kevin M. Hayden; *Applied Biosystems, Framingham, MA*

WOCpm 3:20 **High M/Z Range, High Resolution Coaxial Multiple Reflection ESI-TOFMS;** Melvin A. Park; Ching Wu; Yang Wang; Thomas Dresch; Ulrich Giessmann; *Bruker Daltonics, Inc., Billerica, MA*

WOCpm 3:40 **Design and Construction of a Versatile Gas Chromatography/Electron Monochromator Time-of-Flight Mass Spectrometer (GC/EM TOF MS) System;** Douglas F. Barofsky[1]; Max L. Deinzer[1]; Robert B. Cody[2]; Marc Gonin[3]; Albert J. Schultz[3]; *[1]Oregon State University, Corvallis, OR; [2]JEOL USA Inc., Peabody, MA; [3]Ionwerks Inc., Houston, TX*

WOCpm 4:00 **Orthogonal Injection Matrix-Assisted Laser Desorption/Ionization of Proteins and DNA with UV and IR Lasers;** Maciej Bromirski[1]; Werner Ens[1]; Alexander Loboda[1]; Kenneth G. Standing[1]; Stefan Berkenkamp[2]; Franz Hillenkamp[2]; *[1]University of Manitoba, Winnipeg, Canada; [2]University of Muenster, Muenster, Germany*

WOCpm 4:20 **Hadamard Transform Time-of-Flight Mass Spectrometry Interfaced to Electrospray Ionization of Pressure-Assisted Capillary Electrophoresis**; Joel R. Kimmel[1]; Jose M. Vadillo[1]; Facundo M. Fernandez[1]; Magnus Wetterhall[3]; Nestor Rodriquez[2]; Karin E. Markides[3]; Richard N. Zare[1]; *[1]Dept. of Chemistry, Stanford University, Stanford, CA; [2]Pacific Northwest National Laboratories, Richland, WA; [3]Dept. of Chemistry, Uppsala University, Uppsala, Sweden*

WOCpm 4:40 **Ion Mobility/TOFMS Methods for Parallel Sequencing of Biological Mixtures**; Cherokee S. Hoaglund Hyzer; David E. Clemmer; *Indiana University, Bloomington, IN*

WEDNESDAY AFTERNOON ORAL SESSION WOD
LC/MS: MICROSCALE, Mark R. Emmett, Chair

WODpm 3:00 **Keynote Lecture**; James Jorgenson

WODpm 3:20 **Capillary LC/MS of Peptides with Surface-Modified Monolithic PS-DVB Packing Coupled with an Electrospray Nozzle Chip**; Jack Henion; Xian Huang; Simon Prosser; Tom Corso; Sheng Zhang; Gary Schultz; *Advion BioSciences Inc., Ithaca, NY*

WODpm 3:40 **On-Line Monitoring of Endogenous Neuropeptides by *In Vivo* Microdialysis Capillary LC/ESI/MS/MS**; William E Haskins; Ziqiang Wang; Chris J. Watson; Rebecca R. Rostand; David H. Powell; Robert T. Kennedy; *University of Florida, Gainesville, FL*

WODpm 4:00 **Contrapuntal Strategies for Improving Proteome Coverage with Nanoscale Capillary LC/MS/MS: Variations on a Theme**; Arthur Moseley[1]; Kevin Blackburn[1]; William Burkhart[1]; Roderick Davis[1]; Mary Moyer[1]; Danie Schlatzer[1]; Jim Langridge[2]; Richard Tyldesley[2]; Gary Schultz[3]; Jack Henion[3]; Emine Koc[4]; Linda Spremulli[4]; *[1]GlaxoSmithKline, RTP, NC; [2]Micromass, Altincham, UK; [3]Advanced BioAnalytical Services, Ithaca, NY; [4]University of North Carolina, Chapel Hill, NC*

WODpm 4:20 **Phosphoproteome Analysis of Capacitated Human Sperm Cells**; Scott B. Ficarro; Olga Chertihin; Forest M. White; Jeffrey Shabanowitz; John C. Herr; Pablo Visconti; Donald F. Hunt; *University of Virginia, Charlottesville, VA*

WODpm 4:40 **Comparison of Different Nanoscale Methods for the Analysis of the Nucleolus, a Very Complex Human Organelle**; Jens Andersen[1]; Alexandre V. Podtelejnikov[2]; Henrik Molina[2]; Allan Stensballe[2]; Angus Lamond[3]; Steven P. Gygi[4]; Matthias Mann[1]; *[1]Protein Interaction Laboratory, Odense, Denmark; [2]MDS Proteomics, Odense, Denmark; [3]Department of Biochemistry, Dundee, UK; [4]Harvard Medical School, Boston, MA*

WEDNESDAY AFTERNOON ORAL SESSION WOE
CHARGE PERMUTATION/TRANSFER, Elizabeth Stemmler, Chair

WOEpm 3:00 **Charge Permutation Reactions: Yesterday and Today**; Scott A. McLuckey; *Purdue University, West Lafayette, IN*

WOEpm 3:20 **Ion Chemistry Strategies for the Generation of Transient Uracil Radicals**; Frantisek Turecek; Jill K. Wolken; Erik A. Syrstad; Shetty Vivekananda; *University of Washington, Seattle, WA*

WOEpm 3:40 **The Unimolecular Chemistry of Lithiated vs. Protonated Cytosine Ions and Radicals: Mass Spectral and Computational Investigation**; Michael J. Polce; David A. Modarelli; Chrys Wesdemiotis; *The University of Akron, Akron, OH*

WOEpm 4:00 **The Formation of Gas Phase Zwitterion of Amino Acids in Cyclodextrin Cavities**; Seonghee Ahn; Carlito B. Lebrilla; *University of California, Davis, CA*

WOEpm 4:20 **Fragmentation and Charge Reduction of Solvated Di- and Trivalent Metal Cations in the Gas Phase**; Alexandre A. Shvartsburg; K.W. Michael Siu; *Department of Chemistry, York University, Toronto, ON, Canada*

WOEpm 4:40 **Super-Charging Protein and Peptide Ions Formed by Electrospray Ionization**; Anthony T. Iavarone; John C. Jurchen; Evan R. Williams; *University of California, Berkeley, CA*

WEDNESDAY AFTERNOON ORAL SESSION WOF
MS/MS OF POLYMERS, Scott D. Hanton, Chair

WOFpm 3:00 **MALDI-PSD MS of Modified and Native Poly(propyleneimine) and Poly(amidoamine) Dendrimers**; Tracy D. McCarley; Charles O. Noble, IV; *Louisiana State University, Baton Rouge, LA*

WOFpm 3:20 **The Application of MALDI-TOF Tandem Mass Spectrometry in the Sequencing of Polyester Monomers**; Mark A. Arnould; Chrys Wesdemiotis; *The University of Akron, Akron, OH*

WOFpm 3:40 **MALD/I TOF CID - MS/MS Studies of Polyethylene Glycol**; Andrew J. Hoteling; Kenji Kawaoka; *Eastman Kodak Company, Rochester, NY*

WOFpm 4:00 **Microstructural Studies of Synthetic Polymers Using MALDI-CID: - Experimental Parameters and Information Content;** James H. Scrivens[1]; Anthony T. Jackson[1]; Martin R. Green[2]; Richard Tyldesley[2]; Robert H. Bateman[2]; *[1]ICI Measurement Science Group, Wilton, UK; [2]Micromass Ltd., Manchester, UK*

WOFpm 4:20 **Characterization of Acrylic Telechelic Polymers by Mass Spectrometry**; William J. Simonsick; Atish D. Sen; David J. Aaserud; *DuPont, Philadelphia, PA*

WOFpm 4:40 **Poly(Vinylidene Fluoride): Fragmentation Studies Using an ESI/IT-MS;** Arul Marie[1]; Bruno Ameduri[2]; Jamie Walker[3]; Françoise Fournier[1]; Jean-claude Tabet[1]; *[1]University Pierre et Marie Curie, Paris, France; [2]Ecole Normale Superieure de Chimie, Montpellier, France; [3]Ato Fina, Lyon, France*

PLENARY LECTURE

ThOAam 8:00 **Biomolecular-Isotopic Studies of Biogeochemical Processes**; **John M. Hayes**; *Woods Hole Oceanographic Institute*

THURSDAY MORNING ORAL SESSION ThOA
MS OF EXTRACELLULAR MATRIX & ADHESION MOLECULES, Joseph Zala, Chair

ThOAam 10:15 **Mass Spectrometry of LRR-Proteins in the Extracellular Matrix**; Patrik Önnerfjord; Dick Heinegård; *Lund University, Lund, Sweden*

ThOAam 10:55 **Characterization of MUC Glycopeptides by Nanoelectrospray Low-Energy CID and Electron Capture Dissociation**; Michael Mormann[1]; Iris Meisen[1]; Kristina Hakansson[2]; Terri L. Quenzer[2]; Mark R. Emmett[2]; Alan G. Marshall[2]; Jasna Peter-Katalinic[1]; *[1]Inst. for Medical Physics and Biophysics, Muenster, Germany; [2]National High Magnetic Field Laboratory, Tallahassee, FL*

ThOAam 11:15 **Mass Spectrometric Characterization of Bioactive Heparan Sulfate Neoglycolipid Probes**; Wengang Chai; Christine Leteux; Ten Feizi; Alexander Lawson; *Imperial College School of Medicine, Harrow, UK*

ThOAam 11:35 **Sequence Determination of Chondroitin Polysaccharides via Sequential Enzymatic Digestion and Mass Spectrometric Quantification**; Heather Desaire; Tammy L. Sirich; Julie A. Leary; *University of California, Berkeley, CA*

ThOAam 11:55 **Fine Structure Elucidation of Glycosaminoglycans in the Extracellular Matrix by Electrospray Ionization-Fourier Transform Ion Cyclotron Resonance Tandem Mass Spectrometry**; Joseph E. McClellan; Catherine E. Costello; Joseph Zaia; *Boston University School of Medicine, Boston, MA*

THURSDAY MORNING ORAL SESSION ThOB
TEACHING MS: STRUCTURED & OPEN-ACCESS APPROACHES, Robert Boyd, Chair

ThOBam 10:15 **Keynote Lecture**; William Price, *Marshall University, Huntington, WV*

ThOBam 10:35 **High-Reliability Open Access LC/MS**; Arthur B. Coddington[1]; John Van Antwerp[2]; Michael Jackson[2]; Harri G. Ramjit[1]; *[1]Merck & Co., West Point, PA; [2]Waters Corp., Milford, MA*

ThOBam 10:55 **Teaching the Art of Listening to a Mass Spectrum as an Aid to the Interpretation of Mass Spectral Data**; O. David Sparkman; *University of the Pacific, Stockton, CA*

ThOBam 11:15 **Operation of an Open Access Mass Spec Facility in an Academic Setting**; John Greaves; *University of California, Irvine, CA*

ThOBam 11:35 **The Vitual Mass Spectrometry Laboratory**; Mark E. Bier[1]; Joseph J. Grabowski[2]; *[1]Carnegie Mellon University, Pittsburgh, PA; [2]University of Pittsburgh, Pittsburgh, PA*

ThOBam 11:55 **Open Access Triple Quadrupoles in Pre-Clinical Drug Discovery**; Carmai Seto; Chun Li; Kevin P. Bateman; *Merck Frosst Canada & Co., Kirkland, Canada*

THURSDAY MORNING ORAL SESSION ThOC
MICROFABRICATION/MICROFLUIDICS, Heinrich Köchling, Chair

ThOCam 10:15 **Integrated Sample Preparation and Detection on a Microfluidic Compact Disk (CD) Decreases Detection Limits for Protein Identification by Mass Spectrometry;** Susanne R. Wallenborg; Anders Palm; Anders Hedström; Helene Dérand; Per Andersson; Magnus Gustafsson; *Gyros AB, Uppsala, Sweden*

ThOCam 10:55 **Biomolecule Analysis Using Polymer-Based Microchip Interfaced to Nanoelectrospray Mass Spectrometry**; Zhaojing Meng; Shize Qi; Steven A. Soper; Patrick A. Limbach; *Louisiana State University, Baton Rouge, LA*

ThOCam 11:15 **Improving Mass Spectrometric Sensitivity Using Micro-Fabricated Multiple Electrospray Emitter Arrays**; Keqi Tang; Yuehe Lin; Dean W. Matson; Taeman Kim; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*

ThOCam 11:35 **Application of Microfluidic Devices for Affinity Selection of Target Peptides**; Pierre Thibault[1]; Jianjun Li[1]; Tammy LeRiche[1]; Tammy-Lynn Tremblay[1]; Eric Bonneil[1]; Can Wang[2]; Jed Harrison[2]; *[1]Institute for Biological Sciences, NRCC, Ottawa, Canada; [2]Dept. of Chem., University of Alberta, Edmonton, Canada*

ThOCam 11:55 **On-Chip Microfluidics for Proteomic Analysis by Electrospray Ionization/Mass Spectrometry**; Séverine Le Gac[1]; Christian Druon[2]; Xavier Mélique[2]; Pierre Tabourier[2]; *[1]Université de Lille, Villeneuve Ascq, France; [2]IEMN, Villeneuve Ascq, France*

THURSDAY MORNING ORAL SESSION ThOD
IMAGING BY MS, Rachel Ogorzalek Loo, Chair

ThODam 10:15 **An Ion Trap/Secondary Ion Microprobe**; Peter J. Todd; T. Gregory Schaaff; *Oak Ridge National Laboratory, Oak Ridge, TN*

ThODam 10:35 **An Automated Imaging Internal Laser Desorption Fourier Transform Mass Spectrometer for Surface Analysis**; Paul L. Tremblay; Timothy R. McJunkin; Jill R. Scott; *INEEL, Idaho Falls, ID*

ThODam 10:55 **Laser Ionization Time-of-Flight Mass Spectrometry for the In-depth Profiling of Phosphorus Diffused in Silicon Wafers**; Jose M. Vadillo[1]; Carmen C. Garcia[1]; Javier Ruiz[2]; J. J. Laserna[1]; *[1]University Malaga, Analytical Chemistry, Malaga, Spain; [2]University Malaga, Applied Physics, Malaga, Spain*

ThODam 11:15 **Probing Changes in the Lipid Composition of the Surface of Laser Treated Artist Paints by MALDI-MS**; Oscar F. van den Brink; Stijn Oonk; Gert B. Eijkel; Jaap J. Boon; Ron M. A. Heeren; *FOM - Atomic and Molecular Physics, Amsterdam, The Netherlands*

ThODam 11:35 **Direct MALDI MS Profiling of Proteins in Brain Tissue Sections of Experimental Parkinson's Disease**; Johan Pierson[1]; Jeremy Norris[2]; Per E. Andrén[1]; Richard M. Caprioli[2]; *[1]Uppsala University, Uppsala, Sweden; [2]Vanderbilt University, Nashville, TN*

ThODam 11:55 **MALDI MS Imaging: A Missing Part in the Puzzle of Imaging Techniques**; Markus Stoeckli; Nicolau Beckmann; Rocco Falchetto; Hans-Ulrich Gremlich; Markus Rudin; Dieter Staab; Matthias Staufenbiel; Karl-Heinz Wiederhold; *Novartis Pharma AG, Basel, Switzerland*

THURSDAY MORNING ORAL SESSION ThOE
ISOTOPE RATIO MS, Kevin Yarasheski, Chair

ThOEam 10:15 **First Results of High Precision Position-Specific Isotope Analysis of N and C in an Amino Acid Analogue**; Nabil M.R. Saad; Anthony L. Michaud; J Thomas Brenna; *Cornell University, Ithaca, NY*

ThOEam 10:35 **Rapid Derivatization of Carbohydrates with Minimal Added Carbon for High Precision Isotopic Analysis**; Bassem I. Ziadeh; Anthony Michaud; Betty A. Lewis; J.Thomas Brenna; *Cornell University, Ithaca, NY*

ThOEam 10:55 **Stable Isotopic Characterization of Analgesic Drugs**; John P. Jasper[1]; Francois Fourel[2]; Andrew Eaton[2]; John Morrison[2]; Andy Phillips[2]; *[1]Micromass UK Limited, Manchester, UK; [2]Molecular Isotope Technologies, Niantic, CT*

ThOEam 11:15 **SAXICAB: Software for Automated High-Precision Continuous-Flow Isotope Ratio Mass Spectrometry**; Gavin L. Sacks; Jason T. Sepp; J. Thomas Brenna; *Cornell University, Ithaca, NY*

ThOEam 11:35 **The Chemistry of Silica Gel Ion Emitters**; Glen F. Kessinger; James E. Delmore; *INEEL, Idaho Falls, ID*

ThOEam 11:55 **Linearity Tests for Secondary Electron Multipliers Used in Isotope Ratio Mass Spectrometry**; Stephan Richter[1]; Steven A. Goldberg[1]; Peter B. Mason[1]; Anthony J. Traina[1]; Hans B. Schwieters[2]; *[1]New Brunswick Laboratory, Chicago, IL; [2]Thermo Finnigan MAT, Bremen, Germany*

THURSDAY MORNING ORAL SESSION ThOF
HYDROCARBON & CHEMICAL PROCESSES: FUTURE CHALLENGES, Chang Samuel Hsu, Chair

ThOFam 10:15 **Characterization of Corrosive Compounds in Petroleum Products Using Atmospheric Pressure Ionization/ Mass Spectrometry**; Walter E. Rudzinski[1]; Dora Mendoza[1]; Steve Sassman[1]; Linette Watkins[1]; Chang Hsu[2]; *[1]Southwest Texas State University, San Marcos, TX; [2]Exxon Mobil Research & Engineering Co., Annandale, NJ*

ThOFam 10:35 **The Molecular Weight Distributions of Heavy Petroleum Fractions by Electrospray Mass Spectrometry**; Stilianos, G. Roussis; Richard Proulx; *Imperial Oil, Sarnia, ON, Canada*

ThOFam 10:55 **Recent Advances in Petrochemical Analyses by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Ryan P. Rodgers[1]; Christine A. Hughey[2]; Christopher L. Hendrickson[1]; Alan G. Marshall[1]; Kuangnan Qian[3]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Florida State University, Tallahassee, FL; [3]ExxonMobil Research Engineering, Annandale, NJ*

ThOFam 11:15 **The Advantages of Nonpolar Matrices for Hydrocarbon Analysis by MALDI-MS**; Stephen F. Macha; Patrick A. Limbach; *Louisiana State University, Baton Rouge, LA*

ThOFam 11:35 **Analysis of Combustion Chamber Deposits by ESI-TOF-MS and MADLI-TOF-MS**; John G. Reynolds[1]; Sharon J. Shields[1]; Joseph W. Roos[2]; *[1]Lawrence Livermore National Laboratory, Livermore, CA; [2]Ethyl Corporation, Richmond, VA*

ThOFam 11:55 **Mass Spectrometry of Cluster Grignard Reagents**; Ljudmila A. Tjurina[1]; Eugene N. Nikolaev[1]; Gennadii B. Barkovskii[1]; Marina I. Nikolaeva[2]; Vladimir V. Smirnov[1]; Irina P. Beletskaya[1]; *[1]Moscow State University, Moscow, Russia; [2]Institute for Energ.Prob. of Chem.Phys., Moscow, Russia*

THURSDAY AFTERNOON ORAL SESSION ThOA
PROTEOMICS: MEDICAL APPLICATIONS, Todd D. Williams, Chair

ThOApm 3:00 **Medical Proteomics: Expectations, Realistic and Otherwise**; Mark W. Duncan; *University of Colorado HSC, Denver, CO*

ThOApm 3:20 **Identification and Validation of Cancer Specific Protein Markers**; Yi Gong[1]; Ge Zhou[1]; Hongjun Shu[1]; She Chen[1]; Mike R. Emmert-Buck[3]; Lance R. Liotta[3]; Emanuel F Petricoin III[2]; Philip Taylor[3]; Yingming Zhao[1]; *[1]UT Southwestern Medical School, Dallas, Dallas, TX; [2]Food and Drug Administration, Bethesda, MD; [3]National Cancer Institute, Bethesda, MD*

ThOApm 3:40 **Dupuytren's Disease as a Model Disease for Proteomic Discovery and Characterization;** Bradley J. Thatcher[1]; John Marshal[1]; Jeffery Howard[3]; Scott Weniberger[2]; Bing Gan[3]; *[1]Syn X Pharma, Mississauga, Canada; [2]Ciphergen Biosystems, Fremont, CA; [3]Hand and Upper Limb Center, London, Canada*

ThOApm 4:00 **From Transcriptomics to Mass Spectrometric Proteome Analysis in Clinical Research**; Michael O. Glocker[1]; Marcus Bantscheff[1]; Saleh Ibrahim[2]; Peter Lorenz[1]; Dirk Koczan[2]; Hans-Juergen Thiesen[2]; *[1]Proteome Center Rostock, Rostock, Germany; [2]Institute of Immunology, Rostock, Germany*

ThOApm 4:20 **A Proteomic Approach to Experimental Parkinson's Disease**; Karl Skold[1]; Jonas Astrom[2]; Bengt Bjellqvist[2]; Per E. Andrén[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Amersham Pharmacia Biotech, Uppsala, Sweden*

ThOApm 4:40 **High Sensitivity Proteomic Analysis of Protein Kinase C ε Complexes**; Peipei Ping[1]; Jun Zhang[1]; Michael R. Pisano[2]; David L. Allen[2]; Kelli J. Biedermann[2]; Richard C. Jones[2]; Ricky D. Edmondson[2]; *[1]Dept. of Medicine, Univ. of Louisville, Louisville, KY; [2]Genomic Solutions, Inc, Ann Arbor, MI*

PLENARY LECTURE

ThOApm 5:30 **The Science Behind Art**; Michael Henchman; *Dept. of Chemistry, Brandeis University, Waltham, MA*

THURSDAY AFTERNOON ORAL SESSION ThOB
PROTEIN FOLDING, Carol Robinson, Chair

ThOBpm 3:00 **Elucidating Mechanisms of Protein Folding and Amyloid Formation**; Andrew D. Miranker; *Yale University, Dept. of MB&B, New Haven, CT*

ThOBpm 3:20 **Identification of Folding Intermediates of α/β Barrel Proteins by Hydrogen Exchange and Mass Spectrometry**; Hai Pan; David Smith; *University of Nebraska, Lincoln, NE*

ThOBpm 3:40 **Protein Folding Landscapes and Ligand Binding Probed by ESI/CAD FT ICR MS**; Stephen J. Eyles; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*

ThOBpm 4:00 **Handcuffing and Cross-Examining a Human Heterodimer with Crosslinkers and MS**; Michelle Trester-Zedlitz; Tom W. Muir; Brian T. Chait; *The Rockefeller University, New York, NY*

ThOBpm 4:20 **High Sensitivity Measurements of Protein Stability by H/D Exchange and MALDI Mass Spectrometry**; Michael C. Fitzgerald; Kendall D. Powell; *Duke University, Durham, NC*

ThOBpm 4:40 **Site Specific Amide Hydrogen/Deuterium Exchange in E. coli Thioredoxin and its Alkylated Adducts Measured by Electrospray Ionization Mass Spectrometry**; Moo-Young Kim; Claudia S. Maier; Max L. Deinzer; *Oregon State University, Corvallis, Oregon*

THURSDAY AFTERNOON ORAL SESSION ThOC
COMPUTER APPLICATIONS, David Stranz, Chair

ThOCpm 3:00 **An Architecture for Instrument-Independent LCMS Data Processing with Web-Based Review and Revision of Results**; Mark F. Bean; Qian K. Jin; Steven A. Carr; Mark E. Hemling; *GlaxoSmithKline, King of Prussia, PA*

ThOCpm 3:20 **Development of a LC/MS Database for Automatic Natural Products Deprelication**; Ling He; Min Chu; Ronald Mierzwa; Junling Gao; Ling Xu; Arthur King; Mahesh Patel; *Schering-Plough Corporation, Kenioworth, NJ*

ThOCpm 3:40 **LC-MS Analytical Screening of Drug Candidates Using Visual Basic and Oracle Database for Acquisition, Processing, and SQL Query of Spectra and Chromatogram Information**; Bernard K. Choi; Nathan A. Yates; *Merck Research Laboratories, Rahway, NJ*

ThOCpm 4:00 **Mass Spectrometry and 21 CFR Part 11 Compliance**; Cynthia A. Palmer[1]; Timothy Getek[2]; *[1]Schering-Plough Research Institute, Kenilworth, NJ; [2]Forest Laboratories, Farmingdale, NY*

ThOCpm 4:20 **Potential of Integral Transforms in Processing of LC-MS Data**; Vladimir I. Baranov; Ron Bonner; *Applied Biosystems/MDS SCIEX, Concord, Canada*

ThOCpm 4:40 **Wavelet Compression and De-Noising of MALDI-MS Measurements of Bacteria**; Peter B. Harrington[1]; Aaron Urbas[1]; Kent J. Voorhees[2]; Jon Rees[2]; *[1]Ohio University, Athens, OH; [2]Colorado School of Mines, Golden, CO*

THURSDAY AFTERNOON ORAL SESSION ThOD
FORENSIC APPLICATIONS OF MS, Jehuda Yinon, Chair

ThODpm 3:00 **LC/MS as a Tool for Case Interpretation in Forensic Toxicology**; Maciej J. Bogusz; *King Faisal Specialist Hospital, Riyadh, Saudi Arabia*

ThODpm 3:20 **Improved Sample Identification and Characterization of Toxicological Samples Using Integrated Multi-Spectral Data**; Cozette M. Cuppett; Michael P. Balogh; Mike R. Jackson; *Waters Corporation, Milford, MA*

ThODpm 3:40 **Mass Spectrometric Characterization of Glucuronic Acid Conjugates of Anabolic-Androgenic Steroids and their Metabolites**; Mario Thevis; Georg Opfermann; Wilhelm Schaenzer; *German Sports University, Biochemistry, Cologne, Germany*

ThODpm 4:00 **GC/MS Analysis of Organic Explosives: In-Injection Port Thermal Desorption;** Michael E. Sigman; Ralph H. Ilgner; *Oak Ridge National Laboratory, Oak Ridge, TN*

ThODpm 4:20 **Smokeless Powder Comparison Using HPLC/ES-ITMS**; John A. Mathis; Bruce R. McCord; *Ohio University, Athens, OH*

ThODpm 4:40 **ICP-MS and ID-ICP-MS Methods for the Analysis of Forensic Glass**; Shirly Montero[1]; Jose R. Almirall[1]; Douglas C. Duckworth[2]; Charles K. Bayne[2]; *[1]Florida International University, Miami, FL; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

THURSDAY AFTERNOON ORAL SESSION ThOE
NATURAL PRODUCTS WITH DRUG POTENTIAL,
Randy Julian, Chair

ThOEpm 3:00 **Using ESI-ITMS MS^n Data to Differentiate Procyanidin Structural and Stereoisomers**; Richard C. Fleming; Rebecca M. O'Malley; David F. Fitzpatrick; Bettye Bing; *University of South Florida, Tampa, FL*

ThOEpm 3:20 **LC/MS Analysis of Alkaloids with Antimalarial Activities in Extracts of Peschiera Fuschiaefolia**; Francois Lepine[1]; Sylvain Milot[1]; Rene Morel[2]; *[1]Millenia Hope Inc., Montreal, QC, Canada; [2]INRS-Institut Armand-Frappier, Laval, QC, Canada*

ThOEpm 3:40 **High Throughput Purification and Analysis of Natural Product Compound Libraries**; Lu Zeng; Peadar Cremin; Helena Vervoort; Chris Lee; *Sequoia Sciences, Inc., San Diego, CA*

ThOEpm 4:00 **Characterization of Free Bryostatin-1 and its Intact Complexes with Albumin and Hemoglobin in Models and Patient Serum and Red Cells Using Electrospray Mass Spectrometry;** John Roboz; Lin Deng; Longhua Ma; Nezhat Farr; *Mount Sinai School of Medicine, New York, NY*

ThOEpm 4:20 **Screening for Electrophilic Metabolites of Botanical Extracts Using Pulsed Ultrafiltration and Liquid Chromatography-Tandem Mass Spectrometry**; Benjamin M. Johnson; Richard B. van Breemen; *University of Illinois at Chicago, Chicago, IL*

ThOEpm 4:40 **Characterization of Metabolism Site of Flavan-3-ols by LC ESI MS/MS**; Cécile Cren-Olivé[1]; Bernadette Coddeville[1]; Mohamed Bouktaib[2]; Christian Rolando[1]; *[1]Université de Lille 1, Lille, France; [2]Universite Sidi Mohamed Ben Abdellah, Fès-Atlas, Maroc*

THURSDAY AFTERNOON ORAL SESSION ThOF
ANALYZING HYDROCARBON MATERIALS: NEW APPROACHES TO OLD PROBLEMS, Patrick A. Limbach, Chair

ThOFpm 3:00 **Saturated Hydrocarbon Analysis by Innovative Field Ionization Mass Spectrometry (FIMS);** Chang S. (Sam) Hsu; Gary J. Dechert; *ExxonMobil Research and Engineering Co., Annandale, NJ*

ThOFpm 3:20 **Selective Ionization, Resolution and Chemical Identification of Naphthenic Acids and Neutral Nitrogen Compounds in Heavy Petroleum Crude by Negative Ion Electrospray FT-ICR Mass Spectrometry**; Christine A. Hughey[1]; Ryan P. Rodgers[2]; Christopher L. Hendrickson[2]; Alan G. Marshall[2]; Kuangnan Qian[3]; Winston K. Robbins[3]; *[1]Florida State University, Tallahassee, FL; [2]National High Magnetic Field Laboratory, Tallahassee, FL; [3]ExxonMobil Research Engineering, Annandale, NJ*

ThOFpm 3:40 **MALDI-TOFMS of Crude Oil Fractions Using Nonpolar and Nonpolar Matrices**; Chad L. Robins; Patrick A. Limbach; *Louisiana State University, Baton Rouge, LA*

ThOFpm 4:00 **Pyrolysis - Photoionization Mass Spectrometry of Ethylene-Methyl Acrylate Copolymers**; Frederick J. Cox[1]; Charles N. McEwen[2]; Elisabeth Hauptman[2]; Murray V. Johnston[1]; *[1]University of Delaware, Newark, DE; [2]E.I. duPont de Nemours and Company, Wilmington, DE*

ThOFpm 4:20 **Development of Low-Energy Collision-Induced Dissociation Tandem MS for Polymer Structure Characterization**; Rui Chen; Liang Li; *University of Alberta, Edmonton, Canada*

ThOFpm 4:40 **Rapid Analysis of Soil Samples by Means of Laser Desorption Laser Mass Spectrometry**; Christian Weickhardt; Karen Toennies; *Brandenburg Technical University, Cottbus, Germany*